

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds :

1-2 1-6

exact bonds :

2-3 3-4 4-5 5-6

normalized bonds :

7-8 7-12 8-9 9-10 10-11 11-12

isolated ring systems :

containing 1 : 7 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:CLASS

=>

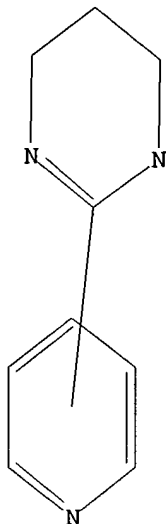
Uploading 10009477 (species).str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam

SAMPLE SEARCH INITIATED 11:39:59 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 19526 TO ITERATE

5.1% PROCESSED 1000 ITERATIONS

10 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
 BATCH **COMPLETE**

PROJECTED ITERATIONS: 382174 TO 398866

PROJECTED ANSWERS: 3067 TO 4743

L2 10 SEA SSS SAM L1

=>

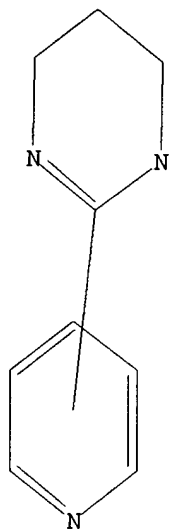
Uploading 10009477 (species).str

L3 STRUCTURE UPLOADED

=> d l3

L3 HAS NO ANSWERS

L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l3 sss sam

SAMPLE SEARCH INITIATED 11:41:11 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 8547 TO ITERATE

11.7% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 165404 TO 176476

PROJECTED ANSWERS: 0 TO 0

L4 0 SEA SSS SAM L3

=>

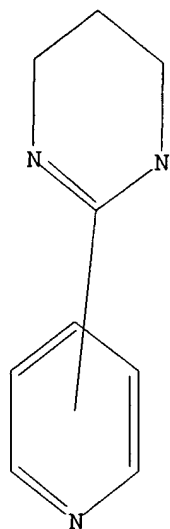
Uploading 10009477 (species).str

L5 STRUCTURE UPLOADED

=> d l5

L5 HAS NO ANSWERS

L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15 sss sam

SAMPLE SEARCH INITIATED 11:42:18 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 19526 TO ITERATE

5.1% PROCESSED 1000 ITERATIONS

0 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 382174 TO 398866

PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s 15 sss ful

FULL SEARCH INITIATED 11:42:30 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 396496 TO ITERATE

100.0% PROCESSED 396496 ITERATIONS

49 ANSWERS

SEARCH TIME: 00.00.05

L7 49 SEA SSS FUL L5

=> s 17

L8 20 L7

=> d 18 1-20 bib,ab,hitstr

L8 ANSWER 1 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 2002:615577 CAPLUS
 DN 137:169536
 TI Preparation of aryl-substituted tetrahydropyrimidines and related
 compounds as melanocortin-4 receptor binding compounds
 IN Maguire, Martin P.; Dai, Mingshi; Vos, Tricia J.
 PA Millennium Pharmaceuticals, Inc., USA
 SO PCT Int. Appl., 228 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002062766	A2	20020815	WO 2002-US3566	20020207
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRAI US 2001-778468 A 20010207 ← I have this case.

OS MARPAT 137:169536

AB Title compds. I [wherein A and B = independently (un)substituted biaryl, (hetero)aryl, Ph, (cyclo)alkyl, (cyclo)alkoxy, alkenyl, alkynyl, OH, acyl(oxy), carbamoyl, amino, thiol, amidino, imino, NO₂, N₃, etc.; L₁ and L₂ = covalent bond or (un)substituted alkyl optionally interrupted by O, S, or N; r = covalent bond, CH, CH₂, CHR₁, CR₁R₂, or H; t = CH, CH₂, CHR₃, CR₃R₄, or H; s = CHR₅, CR₅R₆, or absent; R = H, (un)substituted alkyl, arylalkyl, or heteroalkyl, and may optionally be linked to A, B, L₁, or L₂; R₁-R₆ = independently (un)substituted alkyl, halo, thiol, thioether, thioalkyl, alkoxy, and may be optionally linked to each other to form addnl. ring moieties, e.g., quinoxaliny; or pharmaceutically acceptable salts thereof] were prepd. as melanocortin-4 receptor binding (MC4-R) compds. For example, stirring a soln. of .alpha.-tolunitrile with diisopropylamine and BuLi in hexanes at -78.degree. under nitrogen for 1 h, followed by addn. of HMPA and 1-chloromethylnaphthalene in THF, afforded 2-(2-naphthalen-1-ylethyl)benzonitrile. Heating the benzonitrile with 1,3-diaminopropane in the presence of H₂S at 80.degree. for 72 h gave the tetrahydropyrimidinyl cycloaddn. product II. The latter exhibited exemplary inhibition of MC4-R in a scintillation proximity assay. I are useful for the treatment of disorders assocd. with pigmentation, bones, or wt. loss (no data).

IT **325800-74-6P**, 2-[2-(2-Methoxy-5-nitrobenzylsulfanyl)pyridin-3-yl]-1,4,5,6-tetrahydropyrimidine **325823-83-4P**, 2-[3-(5-Bromo-2-methoxybenzylsulfanyl)pyridin-2-yl]-1,4,5,6-tetrahydropyrimidine **326483-15-2P 447465-95-4P**

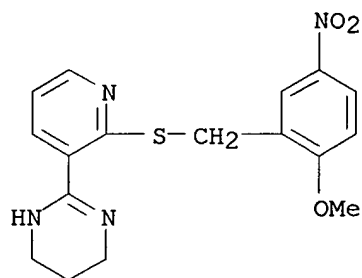
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(MC4-R binding compd.; prepn. of aryl-substituted tetrahydropyrimidines and related compds. as melanocortin-4 receptor binding compds. for treatment of pigmentation, bone, and wt. loss disorders)

RN 325800-74-6 CAPLUS

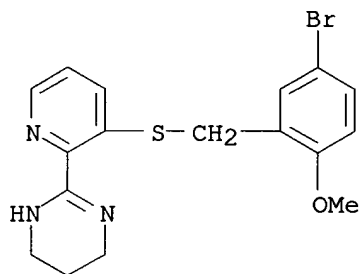
*not
publ.*

CN Pyrimidine, 1,4,5,6-tetrahydro-2-[2-[[2-methoxy-5-nitrophenyl)methyl]thio]-3-pyridinyl]- (9CI) (CA INDEX NAME)



RN 325823-83-4 CAPLUS

CN Pyrimidine, 2-[3-[[5-bromo-2-methoxyphenyl)methyl]thio]-2-pyridinyl]-1,4,5,6-tetrahydro- (9CI) (CA INDEX NAME)



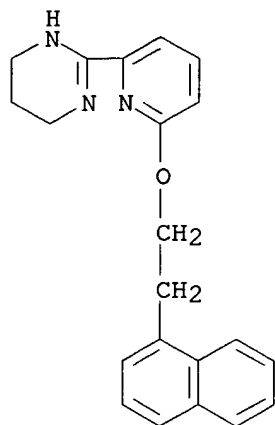
RN 326483-15-2 CAPLUS

CN Formic acid, compd. with 1,4,5,6-tetrahydro-2-[6-[2-(1-naphthalenyl)ethoxy]-2-pyridinyl]pyrimidine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 326483-14-1

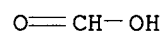
CMF C21 H21 N3 O



CM 2

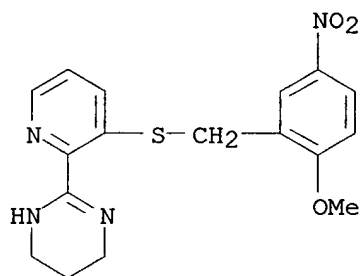
CRN 64-18-6

CMF C H2 O2



RN 447465-95-4 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-2-[3-[[(2-methoxy-5-nitrophenyl)methyl]thio]-2-pyridinyl]-, monohydrobromide (9CI) (CA INDEX NAME)



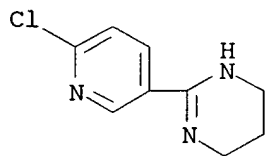
● HBr

L8 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 2001:793434 CAPLUS
 DN 135:339275
 TI Cyclic amidines, nicotinic acetylcholine .alpha.4.beta.2 receptor
 activators containing them, and pharmaceuticals
 IN Imoto, Masahiro; Iwanami, Tatsuya; Akabane, Minako; Tani, Yoshihiro
 PA Suntory, Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 25 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2001302643	A2	20011031	JP 2000-120976	20000421
	WO 2001081334	A2	20011101	WO 2001-JP3378	20010420
	WO 2001081334	A3	20020808		
	W: AU, CA, CN, KR, US				
	RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
PRAI	JP 2000-120976	A	20000421		
OS	MARPAT 135:339275				
AB	The activators, useful for treatment of brain function disorders, contain cyclic amidines I [A1, A2 = H, (un)substituted alkyl, (un)substituted aryl, (un)substituted heterocyclyl; X = (un)substituted C2H4, (un)substituted CH:CH, (un)substituted (CH2)3, (un)substituted CH2CH2NH] or their salts. Trimethylenediamine was cyclocondensed with Et (6-chloro-3-pyridyl)acetate and treated with fumaric acid to give I fumarate (A1 = H, A2 = 6-chloro-3-pyridylmethyl, X = CH:CH), which showed affinity with rat nicotinic acetylcholine .alpha.4.beta.2 receptor with Ki of 29 nM, vs. 1.6 nM, for nicotine. Pharmaceutical formulations contg. I are given.				
IT	371121-78-7P 371121-82-3P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of cyclic amidines as nicotinic acetylcholine .alpha.4.beta.2 receptor activators)				
RN	371121-78-7 CAPLUS				
CN	Pyrimidine, 2-(6-chloro-3-pyridinyl)-1,4,5,6-tetrahydro-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)				

CM 1

CRN 371121-77-6
 CMF C9 H10 Cl N3



CM 2

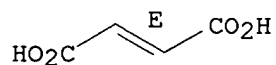
Elected species.

10/009,477 (species)

CRN 110-17-8

CMF C4 H4 O4

Double bond geometry as shown.



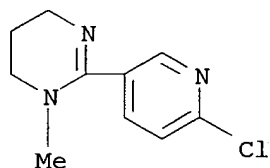
RN 371121-82-3 CAPLUS

CN Pyrimidine, 2-(6-chloro-3-pyridinyl)-1,4,5,6-tetrahydro-1-methyl-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 371121-81-2

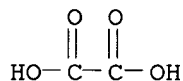
CMF C10 H12 Cl N3



CM 2

CRN 144-62-7

CMF C2 H2 O4



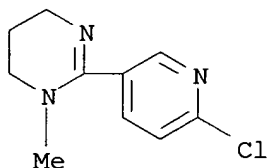
IT 371121-81-2

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

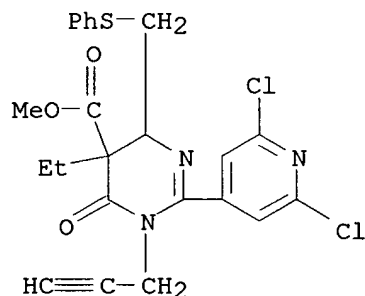
(prepn. of cyclic amidines as nicotinic acetylcholine .alpha.4.beta.2 receptor activators)

RN 371121-81-2 CAPLUS

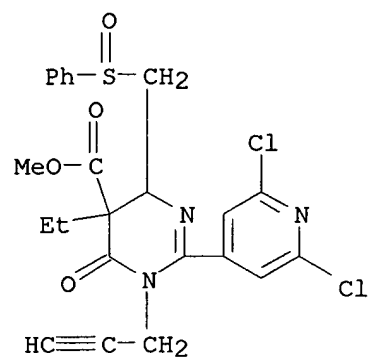
CN Pyrimidine, 2-(6-chloro-3-pyridinyl)-1,4,5,6-tetrahydro-1-methyl- (9CI) (CA INDEX NAME)



L8 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1997:417074 CAPLUS
 DN 127:149117
 TI Synthesis of 2-(2,6-dichloro-4-pyridyl)-3-propargyl-5-ethyl-6-methyl-4(3H)-pyrimidinone, a promising new herbicide
 AU Taylor, Edward C.; Zhou, Ping; Tice, Colin M.; Lidert, Zev; Roemmele, Renee C.
 CS Dep. Chemistry, Princeton Univ., Princeton, NJ, 08544, USA
 SO Tetrahedron Letters (1997), 38(25), 4339-4342
 CODEN: TELEAY; ISSN: 0040-4039
 PB Elsevier
 DT Journal
 LA English
 OS CASREACT 127:149117
 AB A novel synthesis of the title compd. I, a promising new herbicide, is reported which features regioselective carbon, followed by nitrogen, dialkylation of an intermediate dianion, and a tandem one-pot sequence of reactions involving sigmatropic sulfoxide elimination, LiCl-induced demethylation of a carbomethoxy grouping, decarboxylation, and isomerization/aromatization.
 IT **193286-89-4P 193286-90-7P**
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (intermediate in prepn. of (dichloropyridyl)propargylethylmethylpyrimidinone)
 RN 193286-89-4 CAPLUS
 CN 5-Pyrimidinecarboxylic acid, 2-(2,6-dichloro-4-pyridinyl)-5-ethyl-1,4,5,6-tetrahydro-6-oxo-4-[(phenylthio)methyl]-1-(2-propynyl)-, methyl ester (9CI) (CA INDEX NAME)

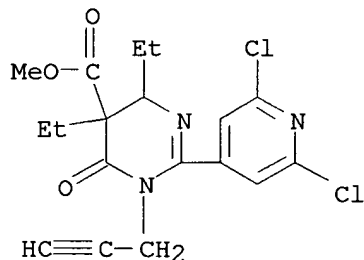


RN 193286-90-7 CAPLUS
 CN 5-Pyrimidinecarboxylic acid, 2-(2,6-dichloro-4-pyridinyl)-5-ethyl-1,4,5,6-tetrahydro-6-oxo-4-[(phenylsulfinyl)methyl]-1-(2-propynyl)-, methyl ester (9CI) (CA INDEX NAME)

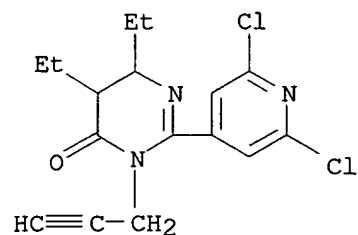


L8 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1996:630487 CAPLUS
 DN 125:275903
 TI Preparation of 2-aryl-5,6-dihydropyrimidin-4-ones as herbicides
 IN Tice, Colin Michael; Bryman, Lois Merle; Roemmele, Renee Caroline
 PA Rohm and Haas Company, USA
 SO Eur. Pat. Appl., 24 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 733622	A1	19960925	EP 1996-301548	19960306
	R: DE, ES, FR, GB, IT				
	US 5629264	A	19970513	US 1995-409293	19950323
	AU 9648005	A1	19961003	AU 1996-48005	19960312
	AU 710045	B2	19990909		
	CA 2171926	AA	19960924	CA 1996-2171926	19960315
	BR 9601059	A	19980106	BR 1996-1059	19960320
	CN 1141292	A	19970129	CN 1996-103157	19960321
	JP 08283245	A2	19961029	JP 1996-91856	19960322
PRAI	US 1995-409293		19950323		
OS	MARPAT 125:275903				
AB	Title compds. [I; R = (hetero)aryl; R3 = (halo)alkenyl, alkoxyalkyl, cyanoalkyl, etc.; R5a, R5b = H, halo, alkyl, alkoxy, etc.; R6a, R6b = H, halo, alkyl, alkoxy, etc.; R5aR6a = (CH2)2-5; X = O or S] were prepd. Thus, 3-ClC6H4C(:NH)NH2 was cyclocondensed with F3CCH:CHCO2Et and the product N-alkylated with HC.tplbond.CCH2Br to give I (R = C6H4Cl-3, R3 = CH2C.tplbond.CH, R5a = R5b = R6b = H, R6a = CF3) which gave 90-100% control of 5 weeds at 1200g/ha preemergent.				
IT	182254-57-5P 182254-58-6P 182254-59-7P 182254-62-2P				
	RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of 2-aryl-5,6-dihydropyrimidin-4-ones as herbicides)				
RN	182254-57-5 CAPLUS				
CN	5-Pyrimidinecarboxylic acid, 2-(2,6-dichloro-4-pyridinyl)-4,5-diethyl-1,4,5,6-tetrahydro-6-oxo-1-(2-propynyl)-, methyl ester (9CI) (CA INDEX NAME)				

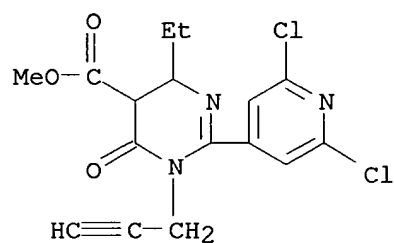


RN 182254-58-6 CAPLUS
 CN 4(3H)-Pyrimidinone, 2-(2,6-dichloro-4-pyridinyl)-5,6-diethyl-5,6-dihydro-3-(2-propynyl)- (9CI) (CA INDEX NAME)



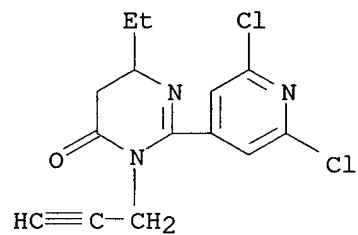
RN 182254-59-7 CAPLUS

CN 5-Pyrimidinecarboxylic acid, 2-(2,6-dichloro-4-pyridinyl)-4-ethyl-1,4,5,6-tetrahydro-6-oxo-1-(2-propynyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 182254-62-2 CAPLUS

CN 4(3H)-Pyrimidinone, 2-(2,6-dichloro-4-pyridinyl)-6-ethyl-5,6-dihydro-3-(2-propynyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1996:625489 CAPLUS
 DN 125:275528
 TI Preparation of carbapenem compounds as antibacterials
 IN Miwa, Tetsuo; Higuchi, Noriko; Soejima, Seizo; Okonogi, Kenji
 PA Takeda Chemical Industries, Ltd., Japan
 SO PCT Int. Appl., 152 pp.
 CODEN: PIXXD2

DT Patent
 LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9626939	A1	19960906	WO 1996-JP509	19960301
	W:	AL, AM, AU, AZ, BB, BG, BR, BY, CA, CN, CZ, EE, GE, HU, IS, KG, KR, KZ, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU			
	RW:	KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
	AU 9648448	A1	19960918	AU 1996-48448	19960301
	JP 09165388	A2	19970624	JP 1996-44424	19960301
PRAI	JP 1995-42765		19950302		
	JP 1995-69343		19950328		
	JP 1995-261371		19951009		
	WO 1996-JP509		19960301		

OS MARPAT 125:275528

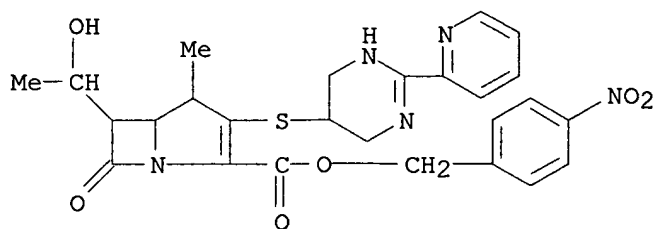
AB Carbapenem compds. I [R1 = (un)substituted lower alkyl group; R2 = H, lower alkyl group; Y = bond, (un)substituted alkylene group; W = Q, Q1; A = (un)hydrogenated pyrimidine ring which may be substituted; X = (un)substituted hetero-atom; X may form a ring, taken together with the ring A-constituent nitrogen atom; X1 = O, S; X2 = NH, O or S; ring A1 may be substituted, provided that, when X2 = NH, X1 = O; R2 = lower alkyl] or their esters or salts, useful as antibacterials, are prepd. Thus, 5-(4-methoxybenzylthio)-2-(methylthio)-1,4,5,6-tetrahydropyrimidine was treated with CF3COOH-anisole and the resulting pyrimidinethiol was reacted with 4-nitrobenzyl (4R,5R,6S)-3-[(diphenylphosphono)oxy]-6-[(R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylate in MeCN contg. diisopropylethylamine to give the title compd. 4-nitrobenzyl (4R,5R,6S)-3-[2-(methylthio)-1,4,5,6-tetrahydropyrimidin-5-ylthio]-6-[(R)-1-hydroxyethyl]-4-methyl-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylate, which was sapond. with NaOH to give sodium (4R,5S,6S)-[(R)-1-hydroxyethyl]-4-methyl-3-[(2-methylthio-1,4,5,6-tetrahydropyrimidin-5-yl)thio]-7-oxo-1-azabicyclo[3.2.0]hept-2-ene-2-carboxylate. In an in vitro study using Muller-Hinton agar medium, this had an IC50 of 0.05.times.106 CFU/mL against Escherichia coli vs. 0.1.times.106 CFU/mL for Imipenem.

IT 182203-13-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
 (prepn. of carbapenem compds. as antibacterials)

RN 182203-13-0 CAPLUS

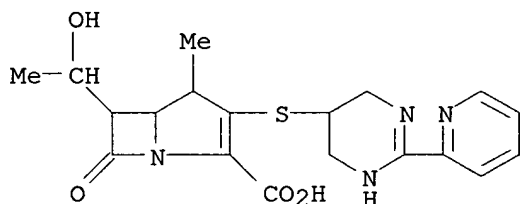
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-7-oxo-3-[[1,4,5,6-tetrahydro-2-(2-pyridinyl)-5-pyrimidinyl]thio]-, (4-nitrophenyl)methyl ester (9CI) (CA INDEX NAME)

IT **182203-15-2P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of carbapenem compds. as antibacterials)

RN 182203-15-2 CAPLUS

CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 6-(1-hydroxyethyl)-4-methyl-7-oxo-3-[[1,4,5,6-tetrahydro-2-(2-pyridinyl)-5-pyrimidinyl]thio]-, monosodium salt (9CI) (CA INDEX NAME)



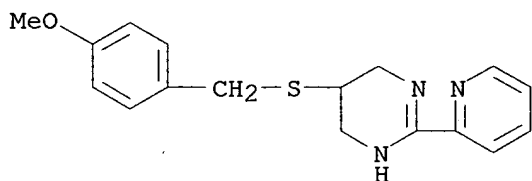
● Na

IT **182204-23-5P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of carbapenem compds. as antibacterials)

RN 182204-23-5 CAPLUS

CN Pyrimidine, 1,4,5,6-tetrahydro-5-[[4-methoxyphenyl)methyl]thio]-2-(2-pyridinyl)- (9CI) (CA INDEX NAME)



L8 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2002 ACS

AN 1991:632273 CAPLUS

DN 115:232273

TI Nitrogen-containing heterocyclic compounds and their optically active isomers

IN Matsumura, Koichi; Mano, Mitsuhiko; Nishimura, Tatsuo; Sugiyama, Yoshio

PA Takeda Chemical Industries, Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

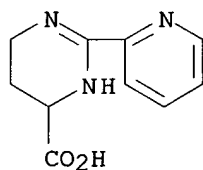
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 03086867	A2	19910411	JP 1990-168795	19900626
PRAI	JP 1989-163482		19890626		

AB Title compds. I or II (R1 = H, C1-18 alkyl, aryl, aralkyl, heterocyclic group; R2 = H, C1-8 alkyl; n = 0-3; R2 = C1-8 alkyl when n = 1 and R1 = H or Me) and their salts and optically active isomers, useful as intermediates for pharmaceuticals, agrochemicals, and liq. crystals, are prepd. Thus, refluxing Me propionimide hydrochloride and 1,4-diaminobutyric acid in MeOH in the presence of NaOMe gave 90% 2-ethyl-1,4,5,6-tetrahydro-4-pyrimidinecarboxylic acid.

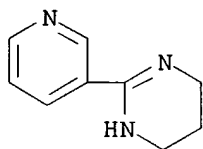
IT **137023-65-5P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of, by condensation of diaminobutyric acid and imide ester)

RN 137023-65-5 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 1,4,5,6-tetrahydro-2-(2-pyridinyl)- (9CI)
 (CA INDEX NAME)

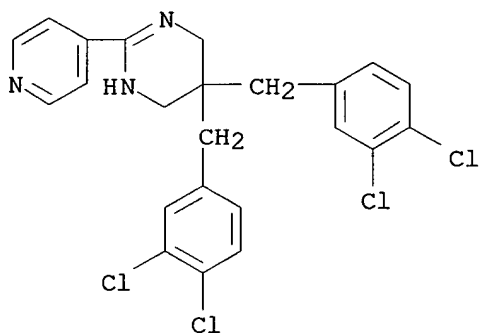


L8 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2002 ACS
AN 1988:32483 CAPLUS
DN 108:32483
TI Effects of nucleus basalis lesions on the muscarinic and nicotinic modulation of [3H]acetylcholine release in the rat cerebral cortex
AU Meyer, Edwin M.; Arendash, Gary W.; Judkins, Jennifer H.; Ying, Lily; Wade, Cathy; Kem, William R.
CS Sch. Med., Univ. Florida, Gainesville, FL, 32610, USA
SO J. Neurochem. (1987), 49(6), 1758-62
CODEN: JONRA9; ISSN: 0022-3042
DT Journal
LA English
AB Adult male rats received unilateral infusions of ibotenic acid (5 .mu.g/.mu.L) in the nucleus basalis magnocellularis (nbm). Two weeks later, cerebral cortical cholinergic markers (choline acetyltransferase activity, high-affinity choline uptake, and coupled acetylcholine (ACh) synthesis) were reduced in synaptosomes prepd. from the lesioned hemispheres compared to contralateral controls. The depolarization-induced release of [3H]ACh from these synaptosomes was also reduced in the lesioned hemispheres, reflecting the reduced synthesis of transmitter. However, the nbm lesions had no effect on the inhibition of release induced by 100 .mu.M oxotremorine. Synaptosomal [3H]ACh release was not altered by nicotine or the nicotinic agonists anabaseine and 2-(3-pyridyl)-1,4,5,6-tetrahydropyrimidine. Nicotine (10-100 .mu.M) did increase [3H]ACh release in control and lesioned hemispheres in cortical minces, but to a similar extent. Apparently, neither muscarinic nor nicotinic receptors modulating ACh release reside on nbm-cholinergic terminals.
IT **112147-36-1**
RL: BIOL (Biological study)
(acetylcholine release response to, in brain cerebral cortex, nucleus basalis in relation to)
RN 112147-36-1 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)



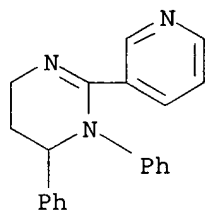
same as #13

L8 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1983:463892 CAPLUS
 DN 99:63892
 TI Appraisals of compounds of diverse chemical classes for capacities to cure infections with sporozoites of *Plasmodium cynomolgi*
 AU Schmidt, L. H.
 CS South. Res. Inst., Kettering-Meyer Lab., Birmingham, AL, USA
 SO Am. J. Trop. Med. Hyg. (1983), 32(2), 231-57
 CODEN: AJTHAB; ISSN: 0002-9637
 DT Journal
 LA English
 AB Comps. of widely diverse structures were appraised for radical curative activity in rhesus monkeys infected with sporozoites of the B strain of *P. cynomolgi*, using an evaluation system that provided a preliminary assessment with from 0.1-1.0 g of compd. and tests against 1 to 5 active infections. None of 32 compds. in a misc. structure category, none of 7 agents of antibiotic origin, none of twelve 1,5-naphthyridines, and none of seven 7-aminoquinolines exhibited curative activity at the largest test doses. One of 12 newly synthesized pyrocatechols appeared to have curative effect. Two of twenty 6-aminoquinolines showed curative effect at or near max. tolerated doses. In contrast, 90 of 174 8-aminoquinolines had curative effects, 18 of the 90 being as active as primaquine, 8 twice as active, and 6 four times as active. There were major disagreements between the above results and those recorded by others in mice inoculated with sporozites of *P. berghei* or *P. yoelii nigeriensis*. These discrepancies were of serious dimensions in evaluations of the 8-aminoquinolines. This, plus previous near flawless performances of *P. cynomolgi* in identifying agents that would cure naturally acquired *P. vivax* infections, led to the suggestion that the abbreviated simian model employed in these studies be used hereafter in primary screening of new agents for radical curative activity.
 IT **80061-38-7**
 RL: BIOL (Biological study)
 (Plasmodium cynomolgi sporozoites infection therapy with)
 RN 80061-38-7 CAPLUS
 CN Pyrimidine, 5,5-bis[(3,4-dichlorophenyl)methyl]-1,4,5,6-tetrahydro-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

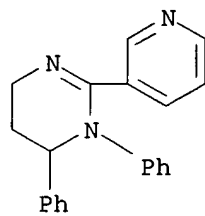


L8 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1983:422491 CAPLUS
 DN 99:22491
 TI 1,4,5,6-Tetrahydropyrimidine derivatives
 IN Gauthier, Jean A.; Jirkovsky, Ivo
 PA Ayerst, McKenna and Harrison Ltd., Can.
 SO U.S., 12 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4379926	A	19830412	US 1978-904124	19780508
OS	CASREACT 99:22491				
AB	Diphenylpyrimidines I (R = alkyl, Ph, 2-furyl, 3-pyridinyl, 2-thienyl, dialkylamino, ZR2; R2 = 1-piperidinyl, 4-morpholinyl; Z = alkylene) were prepd. by cyclization of PhNHCHPhCH2CH2COR (II). Thus, PhNHNH2 108.14, CH2O 30.03, and styrene 104.1 g were cyclocondensed to give 135.9 g 2,3-diphenylpyrazolidine. The latter compd. (133.9 g) was hydrogenated to give 48.4 g PhNHCHPhCH2CH2NH2, which (5.0 g) was benzoylated to give 2.0 g II (R = Ph). This (12.0 g) was cyclized with POCl3 to give 9.3 g I (R = Ph) (III). In rats, 6.25 mg III/kg orally was an effective diuretic.				
IT	86203-86-3P RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. and diuretic activity of)				
RN	86203-86-3 CAPLUS				
CN	Pyrimidine, 1,4,5,6-tetrahydro-1,6-diphenyl-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)				

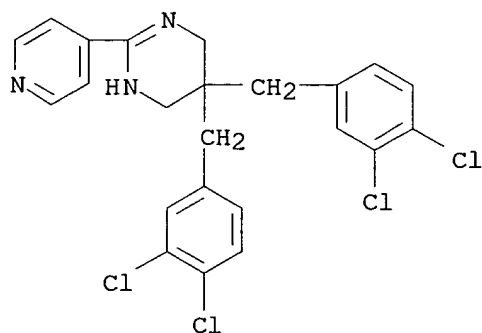


IT **86203-87-4P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 RN 86203-87-4 CAPLUS
 CN Pyrimidine, 1,4,5,6-tetrahydro-1,6-diphenyl-2-(3-pyridinyl)-, monohydrobromide (9CI) (CA INDEX NAME)



● HBr

L8 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1982:62629 CAPLUS
 DN 96:62629
 TI New tissue schizontocidal antimalarial drugs
 AU Davidson, David E., Jr.; Ager, Arba L.; Brown, John L.; Chapple, Frank E.; Whitmire, Richard E.; Rossan, Richard N.
 CS Dep. Parasitol., Walter Reed Army Inst. Res., Washington, DC, 20012, USA
 SO Bull. W. H. O. (1981), 59(3), 463-79
 CODEN: BWHOA6; ISSN: 0366-4996
 DT Journal
 LA English
 AB Over 700 causal prophylactic and radical curative antimalarial drugs have been discovered during the screening of approx. 4000 chem. compds. in rodent and simian malaria models. Causal prophylactic activity in the Plasmodium berghei-rodent model was demonstrated by 10 distinct groups of chems.: 1) tetrahydrofolate dehydrogenase inhibitors, 2) naphthoquinones, 3) dihydroacridinediones, 4) tetrahydrofurans, 5) guanyldrazones, 6) clodidol analogs, 7) quinoline esters, 8) dibenzyltetrahydropyrimidines, 9) 6-aminoquinolines, 10) 8-aminoquinolines. Of the causal prophylactic compds., only the 6- and 8-aminoquinolines were capable of curing persistent exoerythrocytic infections of P. cynomolgi in rhesus monkeys. The 6-aminoquinolines were substantially less active than primaquine. A series of 4-methyl-5-phenoxy-6-methoxy-8-aminoquinolines I (R = F, Cl, OMe, CF₃) were potent blood schizontocides and radical curative drugs. The most active member of this series WR 225448 (I succinate salt, R = CF₃) [80065-56-1], was 5 times more active than primaquine in curing persistent exoerythrocytic infections of P. cynomolgi in rhesus monkeys. As a blood schizontocide, WR 225448 was effective in animal models against P. berghei, P. cynomolgi, P. vivax, and both drug-sensitive and drug-resistant strains of P. falciparum. WR 225448 was also more toxic than primaquine in rats during subacute (28-day) administration.
 IT **80061-38-7**
 RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (antimalarial activity of)
 RN 80061-38-7 CAPLUS
 CN Pyrimidine, 5,5-bis[(3,4-dichlorophenyl)methyl]-1,4,5,6-tetrahydro-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)



Same as #10

L8 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1981:103366 CAPLUS
 DN 94:103366
 TI Urea and amido compounds
 IN Marxer, Adrian
 PA Ciba-Geigy A.-G., Switz.
 SO S. African, 34 pp.
 CODEN: SFXAB

DT Patent
 LA English

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	ZA 7901062	A	19800326	ZA 1979-1062	19790307
	CA 1125759	A1	19820615	CA 1979-321545	19790215
	US 4292429	A	19810929	US 1979-14661	19790223
	FI 7900740	A	19790909	FI 1979-740	19790305
	FI 70708	B	19860626		
	FI 70708	C	19861006		
	EP 4561	A2	19791017	EP 1979-100647	19790305
	EP 4561	B1	19811104		
	EP 4561	A3	19791114		
	R: BE, CH, DE, FR, GB, IT, LU, NL, SE				
	CS 244656	B2	19860814	CS 1979-1460	19790305
	ES 478342	A1	19790516	ES 1979-478342	19790306
	DD 142336	C	19800618	DD 1979-211405	19790306
	PL 116762	B1	19810630	PL 1979-213924	19790306
	PL 123150	B1	19820930	PL 1979-221681	19790306
	IL 56797	A1	19820930	IL 1979-56797	19790306
	DK 7900952	A	19790909	DK 1979-952	19790307
	NO 7900765	A	19790911	NO 1979-765	19790307
	NO 152606	B	19850715		
	NO 152606	C	19851023		
	AU 7944900	A1	19790913	AU 1979-44900	19790307
	AU 531006	B2	19830804		
	AT 7901710	A	19810315	AT 1979-1710	19790307
	AT 364375	B	19811012		
	SU 845779	A3	19810707	SU 1979-2733999	19790307
	HU 25271	O	19830628	HU 1979-CI1920	19790307
	HU 182940	B	19840328		
	JP 54125668	A2	19790929	JP 1979-26245	19790308
	JP 62009109	B4	19870226		
	SU 923367	A3	19820423	SU 1980-2872253	19800118
	AT 8003951	A	19810515	AT 1980-3951	19800730
	AT 365179	B	19811228		
	US 4420619	A	19831213	US 1981-247427	19810325
	CS 244700	B2	19860814	CS 1984-8407	19841105
PRAI	CH 1978-2519		19780308		
	US 1979-14661		19790223		
	CS 1979-1460		19790305		
	AT 1979-1710		19790307		

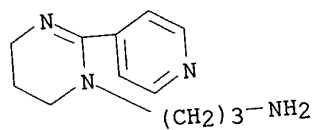
AB The antitumor (no data) compds. I (R = aryl, arylamino, aralkyl, arylaminoalkyl; R1 = aryl, arylamino; X = O, S; X1 = alkylene n = 1, 2) were prep'd. Thus, 2,6-Cl₂C₆H₃NHCH₂CN was treated with HN(CH₂CH₂NH₂)₂ to give II (R₂ = H), which was treated with 4-MeC₆H₄NCO to give II (R₂ = CONHC₆H₄Me-4).

IT 73998-75-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

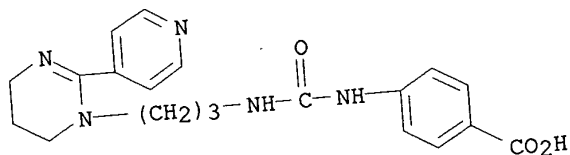
10/009,477 (species)

(prepn. and reaction of, with isocyanates)
RN 73998-75-1 CAPLUS
CN 1(4H)-Pyrimidinepropanamine, 5,6-dihydro-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

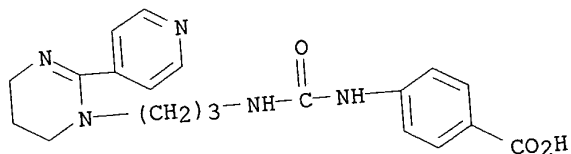


IT 73998-73-9P 76692-14-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 73998-73-9 CAPLUS
CN Benzoic acid, 4-[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



RN 76692-14-3 CAPLUS
CN Benzoic acid, 4-[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L8 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1980:446666 CAPLUS
 DN 93:46666
 TI Process for the preparation of novel imidazole urea and amido compounds
 IN Marxer, Adrian
 PA Ciba-Geigy A.-G., Switz.
 SO Brit. UK Pat. Appl., 14 pp.
 CODEN: BAXXDU
 DT Patent
 LA English
 FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	GB 2016011	A	19790919	GB 1979-8098	19790307
	GB 2016011	B2	19820825		
	CA 1125759	A1	19820615	CA 1979-321545	19790215
	US 4292429	A	19810929	US 1979-14661	19790223
	FI 7900740	A	19790909	FI 1979-740	19790305
	FI 70708	B	19860626		
	FI 70708	C	19861006		
	EP 4561	A2	19791017	EP 1979-100647	19790305
	EP 4561	B1	19811104		
	EP 4561	A3	19791114		
	R: BE, CH, DE, FR, GB, IT, LU, NL, SE				
	CS 244656	B2	19860814	CS 1979-1460	19790305
	ES 478342	A1	19790516	ES 1979-478342	19790306
	DD 142336	C	19800618	DD 1979-211405	19790306
	PL 116762	B1	19810630	PL 1979-213924	19790306
	PL 123150	B1	19820930	PL 1979-221681	19790306
	IL 56797	A1	19820930	IL 1979-56797	19790306
	DK 7900952	A	19790909	DK 1979-952	19790307
	NO 7900765	A	19790911	NO 1979-765	19790307
	NO 152606	B	19850715		
	NO 152606	C	19851023		
	AU 7944900	A1	19790913	AU 1979-44900	19790307
	AU 531006	B2	19830804		
	AT 7901710	A	19810315	AT 1979-1710	19790307
	AT 364375	B	19811012		
	SU 845779	A3	19810707	SU 1979-2733999	19790307
	HU 25271	O	19830628	HU 1979-CI1920	19790307
	HU 182940	B	19840328		
	JP 54125668	A2	19790929	JP 1979-26245	19790308
	JP 62009109	B4	19870226		
	SU 923367	A3	19820423	SU 1980-2872253	19800118
	AT 8003951	A	19810515	AT 1980-3951	19800730
	AT 365179	B	19811228		
	US 4420619	A	19831213	US 1981-247427	19810325
	CS 244700	B2	19860814	CS 1984-8407	19841105
PRAI	CH 1978-2519		19780308		
	US 1979-14661		19790223		
	CS 1979-1460		19790305		
	AT 1979-1710		19790307		

AB Ureas and amides I (R, R2 = monocyclic, carbocyclic aryl or heteroaryl; R1 = H, alkyl; n = 0, 1; m = 0, 1, 2; x = 1, 2; Z = alkylene having 2-3 C atoms in the linear chain; Z1 = O, S; Z2 = imino, bond) and I salts were prep'd. E.g., 1-[2-[2-(2,6-dichloroanilinomethyl)-2-imidazolin-1-yl]ethyl]-3-(p-tolyl)urea was prep'd. by stirring 1-aminoethyl-2-(2,6-dichloroanilinomethyl)-2-imidazoline with p-MeC6H4NCO in PhMe at

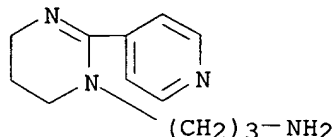
90.degree. for 3 h. I have a powerful action against tumors; their activities were assessed against respiratory carcinomas in golden hamsters and the Ehrlich ascites carcinoma in mice. They are particularly valuable for the treatment of bronchial carcinomas. Compns. contg. I are described.

IT **73998-75-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and addn. reaction of, with aryl isocyanate)

RN 73998-75-1 CAPLUS

CN 1(4H)-Pyrimidinepropanamine, 5,6-dihydro-2-(4-pyridinyl)- (9CI) (CA INDEX NAME)

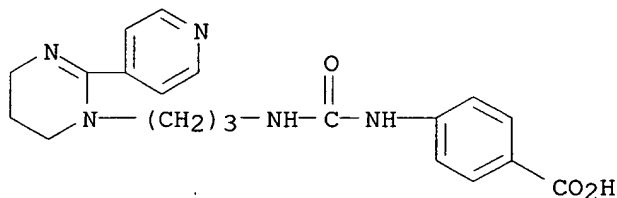


IT **73998-73-9P 73998-74-0P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of, as neoplasm inhibitor)

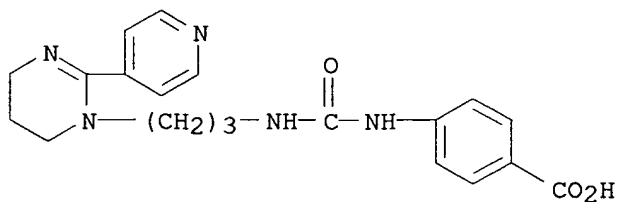
RN 73998-73-9 CAPLUS

CN Benzoic acid, 4-[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]- (9CI) (CA INDEX NAME)



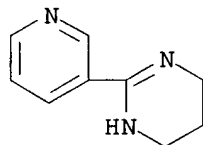
RN 73998-74-0 CAPLUS

CN Benzoic acid, 4-[[[3-[5,6-dihydro-2-(4-pyridinyl)-1(4H)-pyrimidinyl]propyl]amino]carbonyl]amino]-, hydrochloride (9CI) (CA INDEX NAME)



●x HCl

L8 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2002 ACS
AN 1972:429705 CAPLUS
DN 77:29705
TI Actions of some muscarinic and nicotinic agonists on the Retzius cells of the leech
AU Woodruff, Geoffrey N.; Walker, Robert James; Newton, Lynne C.
CS Dep. Physiol. Biochem., Univ. Southampton, Southampton, Engl.
SO Comp. Gen. Pharmacol. (1971), 2(5), 106-17
CODEN: CPGPAY
DT Journal
LA English
AB Twenty-eight acetylcholine analogs, nicotinic and muscarinic agonists, and acetylenic compds. were tested on Retzius cells of the leech (*Hirudo medicinalis*) nerve cord. Generally the acetylcholine analogs and nicotinic agonists were powerful stimulants, causing depolarization with an increase in the rate of firing of action potentials, whereas the muscarinic agonists usually caused hyperpolarization and inhibition of neurons when added in threshold amts. and excitation when added in relatively large amts. Carbachol [51-83-2] and 2-(3-pyridyl)-1,4,5,6-tetrahydropyrimidine-HCl (I) [35059-05-3] were the most potent stimulants, and [4-(m-chlorophenylcarbamoyloxy)-2-butynyl]trimethylammonium chloride (II) [55-45-8] was the most potent inhibitor.
IT **35059-05-3**
RL: PRP (Properties)
(nerve Retzius cell of leech in response to)
RN 35059-05-3 CAPLUS
CN Pyrimidine, 1,4,5,6-tetrahydro-2-(3-pyridinyl)-, monohydrochloride (9CI)
(CA INDEX NAME)



● HCl

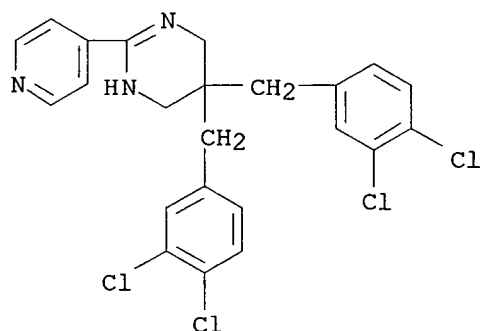
L8 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2002 ACS
 AN 1970:425515 CAPLUS
 DN 73:25515
 TI Tetrahydropyrimidines active against protozoa
 PA Farbwerke Hoechst A.-G.
 SO Fr. Demande, 20 pp.
 CODEN: FRXXBL
 DT Patent
 LA French
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2007450	A1	19700109	FR 1969-11419	19690414
PRAI	DE 1967-1770208		19680413		

AB I (R = 4-pyridyl, 4-sulfamoylphenyl, 4-nitrophenyl, 3-pyridyl, 3-chloro-4-nitrophenyl, 4-cyanophenyl, or a similar group; R1 = 3,4-dichlorobenzyl or 2,4-dichlorobenzyl), and their HCl, maleate, and oxalate salts, are prepd. The compds. exhibit mild activity against protozoa such as Plasmodium berghei and Babesia rodhaini. The compds. are prepd., for example, by the treatment of compds. such as 2,2-bis(3,4-dichlorobenzyl)-1,3-diaminopropane with isonicotinic acid or a similar compd. in aq. HCl.

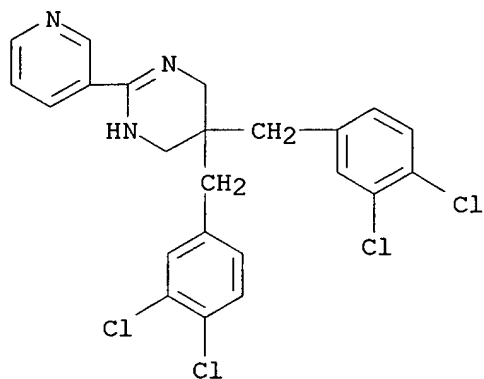
IT **27337-17-3P 27337-19-5P 27338-48-3P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 27337-17-3 CAPLUS
 CN Pyrimidine, 5,5-bis(3,4-dichlorobenzyl)-1,4,5,6-tetrahydro-2-(4-pyridyl)-, dihydrochloride (8CI) (CA INDEX NAME)



●2 HCl

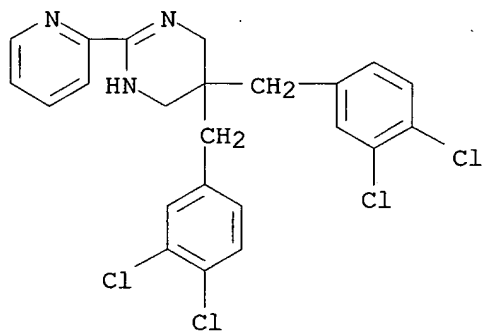
RN 27337-19-5 CAPLUS
 CN Pyrimidine, 5,5-bis(3,4-dichlorobenzyl)-1,4,5,6-tetrahydro-2-(3-pyridyl)-, dihydrochloride (8CI) (CA INDEX NAME)



● 2 HCl

RN 27338-48-3 CAPLUS

CN Pyrimidine, 5,5-bis(3,4-dichlorobenzyl)-1,4,5,6-tetrahydro-2-(2-pyridyl)-, hydrochloride (8CI) (CA INDEX NAME)



● x HCl

10/009,477 (species)

=> d his

(FILE 'HOME' ENTERED AT 11:39:29 ON 24 SEP 2002)

FILE 'REGISTRY' ENTERED AT 11:39:34 ON 24 SEP 2002

L1 STRUCTURE UPLOADED
L2 10 S L1 SSS SAM
L3 STRUCTURE UPLOADED
L4 0 S L3 SSS SAM
L5 STRUCTURE UPLOADED
L6 0 S L5 SSS SAM
L7 49 S L5 SSS FUL

FILE 'CAPLUS' ENTERED AT 11:42:43 ON 24 SEP 2002

L8 20 S L7

FILE 'CAOLD' ENTERED AT 11:43:39 ON 24 SEP 2002

=> s 17

L9 0 L7

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.38

230.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

0.00

-12.39

STN INTERNATIONAL LOGOFF AT 11:43:53 ON 24 SEP 2002